NIST-GCR-91-588

# Compartment Fire Combustion Dynamics

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U.S. DEPARTMENT OF COMMERCE
National Institute of Standards
and Technology
Building and Fire Research Laboratory
Gaithersburg, MD 20899

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## Notice

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# COMPARTMENT FIRE COMBUSTION DYNAMICS

## NIST/CFR GRANT NO. 60NANB8D0829

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## ABSTRACT

As most fire fatalities are the result of exposure to toxic products of combustion, it is essential that methods be devised to evaluate the toxic hazards posed by specific materials in varying building designs. While toxic products are produced during smoldering and open burning combustion modes, the rate of generation of toxic products of incomplete combustion is greatest under conditions where the compartment flow dynamics create oxygen deficient combustion conditions.

This three year investigation will experimentally 1) determine the effect of realistic compartment fire flows on species generation rates and their correlation with equivalence ratio, 2) establish major toxic gas and smoke generation rates for important fuels such as PMMA, wood and TDI-based polyurethane, and 3) determine the efficiency of external flames in destroying major toxic gases produced within the compartment under oxygen deficient compartment fire combustion.

The apparatus that has been built for this investigation includes a 1.2m x 1.2m x 1.5m compartment with two ventilation paths; a normal window style exhaust vent, and a ducted air inlet vent. Separation of the two flows allows a relatively simple measurement of the air inflow, while leaving the exhaust flow dynamics undisturbed. Exhaust from the compartment is collected by a hood system instrumented to allow the measurement of gas and smoke generation rates. This system allows direct measurement of air and fuel supply rates as well as species generation rates.

Hexane-fueled fires have been burned in the compartment resulting in a two layer system as verified by temperature and species concentration measurements. Measurements include species yield, fuel volatilization rate, air entrainment rate and temperature profiles. Correlations between species yield and overall equivalence ratio agree well with Beyler's results [1,2]. The correlation exhibits a two-value function with a transition region between equivalence ratios of 1 and approximately 1.8. The transition from an overventilated (equivalence ratio below one) to an underventilated fire condition is marked by several characteristics: 1) a sharp rise in CO and $CO_2$ concentrations in the upper layer, 2) a sharp decrease in $O_2$ concentration in the upper layer and 3) sustained external burning.

Initial experiments of PMMA-fueled fires have also been conducted. Similar to the hexane fires CO concentrations for overventilated fires are below 0.05%. The PMMA fires show similar results as compared to the under- to overventilated transition in hexane-fueled fires.

## INTRODUCTION

This report summarizes the first two years of a research effort directed toward understanding the generation and spread of toxic gases, particularly carbon monoxide, in realistic compartment fires. As most fire fatalities are the result of exposure to toxic products of combustion, it is essential that methods be devised to evaluate the toxic hazards posed by specific materials in varying building designs. While toxic products are produced during both smoldering and open combustion modes, the rate of generation of toxic products of incomplete combustion, such as carbon monoxide, is greatest under conditions where compartment flow dynamics create oxygen deficient combustion.

Although some features of compartment fire combustion dynamics have been understood for decades, many others have received little attention. In particular, the effect of the compartment on combustion efficiency and toxic gas production has not received attention commensurate with its practical importance. The efficiency of external flames at compartment vents in destroying toxic gases produced in the compartment has not been studied.

Most compartment fire studies to date have not focused on the combustion dynamics themselves. The internal heat release rate is most often simply related to the opening factor, $Ah^{1/2}$. While this approach has been very successful for some applications such as fire resistance calculations, a more detailed understanding of the combustion dynamics is required to address the problems noted above.

The current three year research effort is designed to experimentally 1) determine the effects of realistic fire flows on species generation rates and their correlation with equivalence ratio, 2) establish major toxic gas (especially CO and HCN) and smoke generation rates for important fuels such as PMMA, wood and TDI-based polyurethane, and 3) determine the efficiency of external flames in destroying major toxic gases produced within the compartment under oxygen deficient compartment fire combustion.

## BACKGROUND AND MOTIVATION

While fairly extensive measurements of toxic species production have been made for flaming combustion in an "open burning" mode, it can be shown that most often oxygen depletion and thermal hazards dominate over carbon monoxide under these conditions.

Toxic gas production has been investigated under fuel-rich two layer conditions by Beyler [1,2], Tewarson [3], and Morikawa and Yanai [4]. It has been well established that carbon monoxide yields are significantly increased in this combustion mode over that observed under fuel-lean conditions. It can be shown that under these combustion conditions carbon monoxide is generally a greater hazard than oxygen depletion. The work to date in this area can be categorized into two groups: basic research using highly simplified physical models [1,2], and exploratory research in more realistic compartments with incomplete instrumentation and minimal control of variables [3,4].

The more basic investigations by Beyler were performed with partial support from NBS [1,2] (Grant #60NANB4D0010). Experiments were made in a hood configuration which did not allow a number of compartment effects to operate. The configuration allowed direct measurements of the required physical and chemical variables. However, wall plumes and layer mixing effects were absent and no instabilities were observable. While this was desirable for initial investigations, it is important to evaluate the correlational methods developed in those studies in more realistic compartment fire environments.

The analysis performed by Tewarson [3] was based on data collected in earlier compartment fire experiments in which carbon monoxide concentrations were measured. These experiments were not designed to determine the total CO production rate. No direct measurements of vent flows were made and the quality of the gas analysis is suspect [2]. The quality of the data and the assumptions required to allow the analysis to be performed severely limited the analysis. Nonetheless, the analysis is generally in agreement with the hood studies.

The experiments of Morikawa and Yanai [4] were performed under forced convection conditions in a room with a representative mixture of materials commonly found in buildings. The combustion was largely under fuel-rich conditions and the results indicated that carbon monoxide was the principal though not the only toxic gas of importance. Unfortunately, there is evidence in their paper to indicate that under some conditions the gas sampling was done in the flaming region. This type of sampling, which was also found to have been used in some of the experiments analyzed by Tewarson, generally results in incorrectly high concentrations of products of incomplete combustion, most notably carbon monoxide [2].

In general, good progress has been made in exploring toxic species generation rates under fuel-rich conditions. Hazards due to toxic products have been clearly identified to be worse than those generated in fuel-lean conditions. Fire studies in well controlled hood experiments show that the generation of species is well correlated by the equivalence ratio.

To date no systematic, well-controlled and instrumented compartment fire tests have been reported which examine the effects that compartment fire flows might exert on the quality of species yield correlations with equivalence ratio. Of equal importance, no studies have examined the efficiency of external flames in destroying products of incomplete combustion generated in the compartment.

## RESEARCH PLAN

Experiments are performed in a compartment designed and instrumented to allow direct measurement of all physical and chemical quantities required for evaluation of species and smoke production, and equivalence ratio. The apparatus is fully described below.

The apparatus allows the direct measurement of the fuel-to-air ratio in a compartment fire environment. Direct determination of the yields of gaseous products of combustion and of the specific extinction cross section is possible over a wide range of fuel-to-air ratios for any material that can be burned in a compartment fire experiment. The scale of the experiment insures that the flames will be fully turbulent.

The experimental design utilizes two ventilation paths; a normal window style exhaust vent, and a ducted air inlet vent. Separation of the two flows allows a relatively simple measurement of the air inflow, while leaving the exhaust flow dynamics undisturbed.

The 1.2m x 1.2m x 1.5m compartment is similar to that used by Bullen and Thomas [5], with the necessary modifications to allow separate inlet and outlet flows. The apparatus is shown in Figure 1. Exhaust vents up to 0.5m x 0.5m are possible and inflows are provided through a 0.3m circular duct. Inlet flow is measured by a single point heat transfer based velocity probe. This type of system avoids unacceptable pressure losses associated with orifice meters and is ideal for flow velocities on the order of 0-3m/s. The exhaust vent is sized for each fire such that there is only outflow of combustion products. Therefore, the air entrainment rate is made solely by the velocity probe. As compared to most

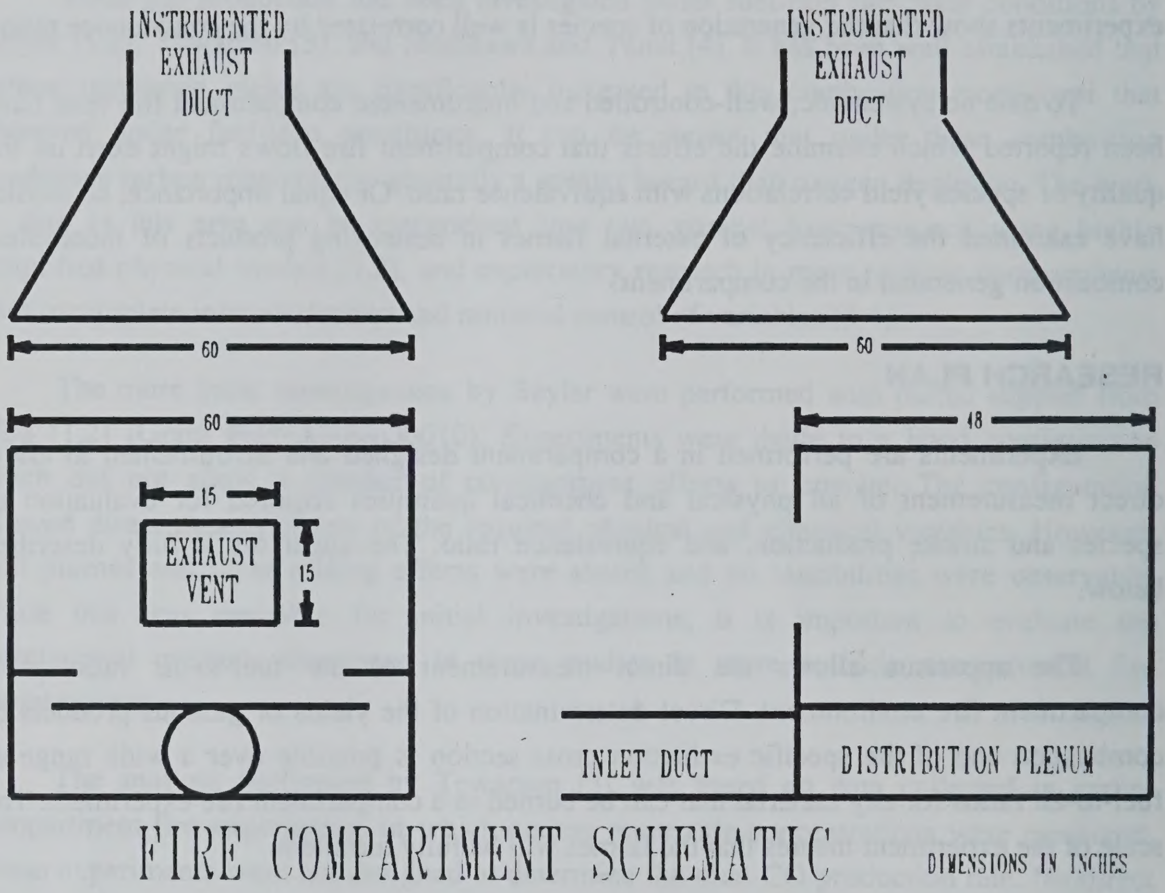

INSTRUMENTED EXHAUST DUCT
INSTRUMENTED EXHAUST DUCT
60
60
60
48
15
EXHAUST VENT
15
INLET DUCT
DISTRIBUTION PLENUM
FIRE COMPARTMENT SCHEMATIC
DIMENSIONS IN INCHES

Figure 1. Fire compartment schematic.

compartment fire testing, the entrainment rate measurement does not rely on the use of the ventilation parameter $Ah^{1/2}$, where A is the vent area and h is the vent height.

The inlet duct is approximately three meters long to allow some development of the flow without unacceptable friction losses. The duct supplies a plenum below the compartment and flow into the compartment is from inlets on the ends of the compartment. The fuel load cell is within the plenum space to provide protection from the compartment environment and afford some air cooling.

The fuel is burned in the center of the compartment approximately 2.5cm from the floor. Hexane is burned in an aluminum pan which is supported by the load cell via an extension piece through the floor. The fuel volatilization rate along with the air entrainment rate afford a direct measurement of the overall plume equivalence ratio.

The natural exhaust flow is collected by a hood specifically designed for experiments of this type and scale. The hood system is capable of handling the exhaust flows for heat release rates of up to 400kW. The exhaust system is instrumented with an orifice meter and a gas sampling probe and will be instrumented with smoke obscuration instrumentation which allows the measurement of the rate of generation of products of combustion. The clearance between the exhaust vent and the hood will allow the study of external flames. Probe sampling of the gases within the compartment is also provided. For all experiments discussed in this report, sampling is performed with an uncooled stainless steel probe. The probe is centered in the exhaust vent 12 cm inside the compartment.

Based on previous work by Beyler [6] it is possible to determine the conditions under which external combustion will occur. The experimental apparatus will allow the direct investigation of the efficiency of the vent flame in destroying toxic gases produced by the substantially incomplete combustion within the compartment. External as well as corridor type flames will be investigated.

## FIRST YEAR ACCOMPLISHMENTS

### Equipment Acquisition

Several new pieces of equipment have been specified and obtained for this project. This equipment includes a high flow, high temperature exhaust blower for the test facility, a high accuracy, low flow velocity measuring probe and a high accuracy differential manometer. All three of these items were purchased with money from the NIST grant. In addition, a Fourier Transform Infrared Analyzer (FTIR), and new carbon monoxide (CO) and carbon dioxide ($CO_2$) Non-Dispersive Infrared Analyzers (NDIRs) were obtained for use in this project with money provide by the Department of Mechanical Engineering at VPI&SU. This equipment was provided for the project in addition to the formal cost-sharing in the original proposal.

The high flow, high temperature exhaust blower has been used to upgrade the current hazardous test facility to handle the exhaust from the fire test compartment. A new blower was required which would handle the large flow rates and high temperatures associated with the fire compartment exhaust. Integral to this exhaust system is an orifice plate for volumetric flow rate measurement. The high accuracy differential manometer will be used with this orifice meter to obtain air flow rates in the exhaust. Since sampling of chemical species will be made in the exhaust, it is important to know the flow rate so that production rates of the various species can be obtained. The low velocity probe is used to measure flow into the test compartment without significant pressure drop. Since this probe measures linear velocity, it must be calibrated against known volumetric flow rates. This calibration was obtained by the use of a previously calibrated low velocity wind tunnel.

The FTIR analyzer and the two NDIR analyzers will be used to measure production rates of chemical species including CO, $CO_2$, HCN and HCl. The analyzers have been specified so that they can be used to analyze samples directly from the compartment or the more dilute samples obtained from the exhaust.

All three analyzer have been received, installed and calibrated. Sample gas mixture indicative of likely fire products have been obtained for calibration of the analyzer for toxic gases likely to be observed. These mixtures include CO, $CO_2$, HCN and HCl. A schematic of the sampling system is shown in Figure 2. The sampling system has two sample probes; one is used for extracting samples from the compartment, the other is used for extracting diluted samples from the exhaust duct. For either sample, the gases are run through a cold trap to remove water and are then sampled by the various analyzers. However, in the case of hydrocarbon measurements, the sample is maintained hot and no water is removed prior to analysis. In addition, provisions for making smoke measurements in the exhaust duct have been made using a light attenuation technique.

## Facilities Development

Renovation of the test facility to be used for this project was completed. The test facility being used for this project is a hazardous test facility previously used for solid rocket propellant testing. A schematic of this facility, which is remote from the main campus, is shown in Figure 3. The facility consists of a 10 foot cube, concrete block test

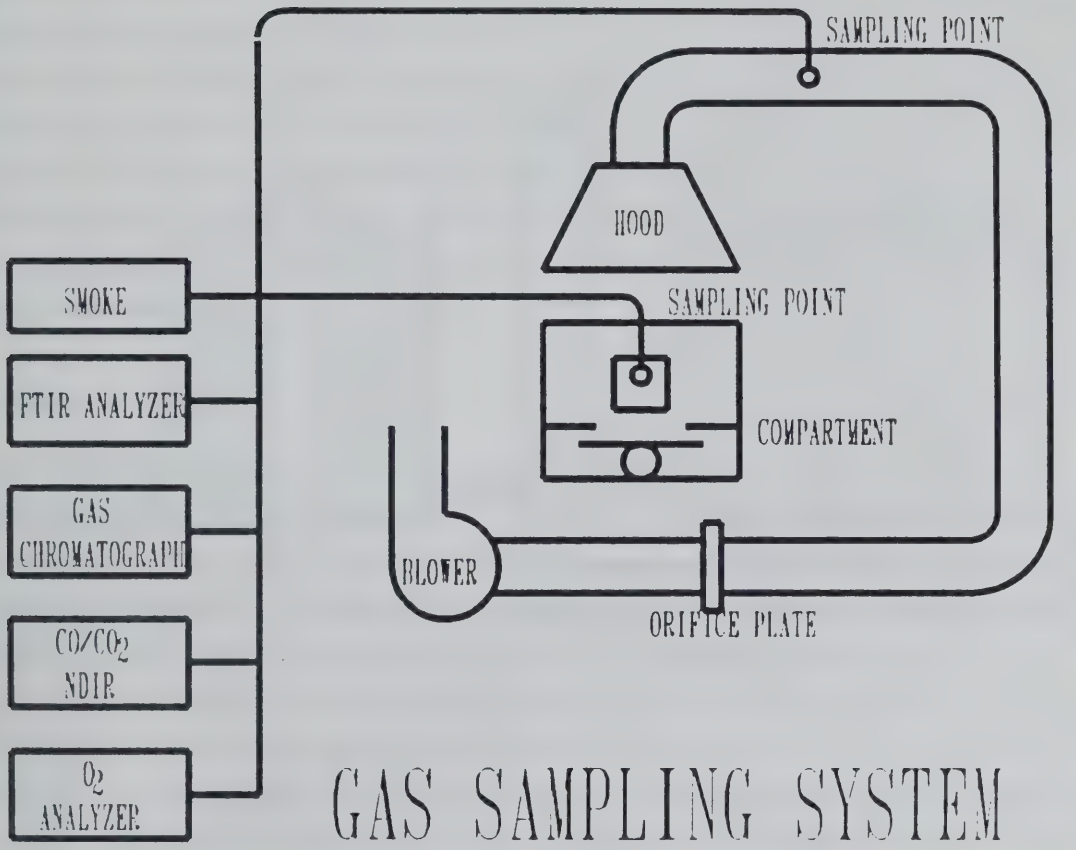


Figure 2. Gas sampling system schematic.

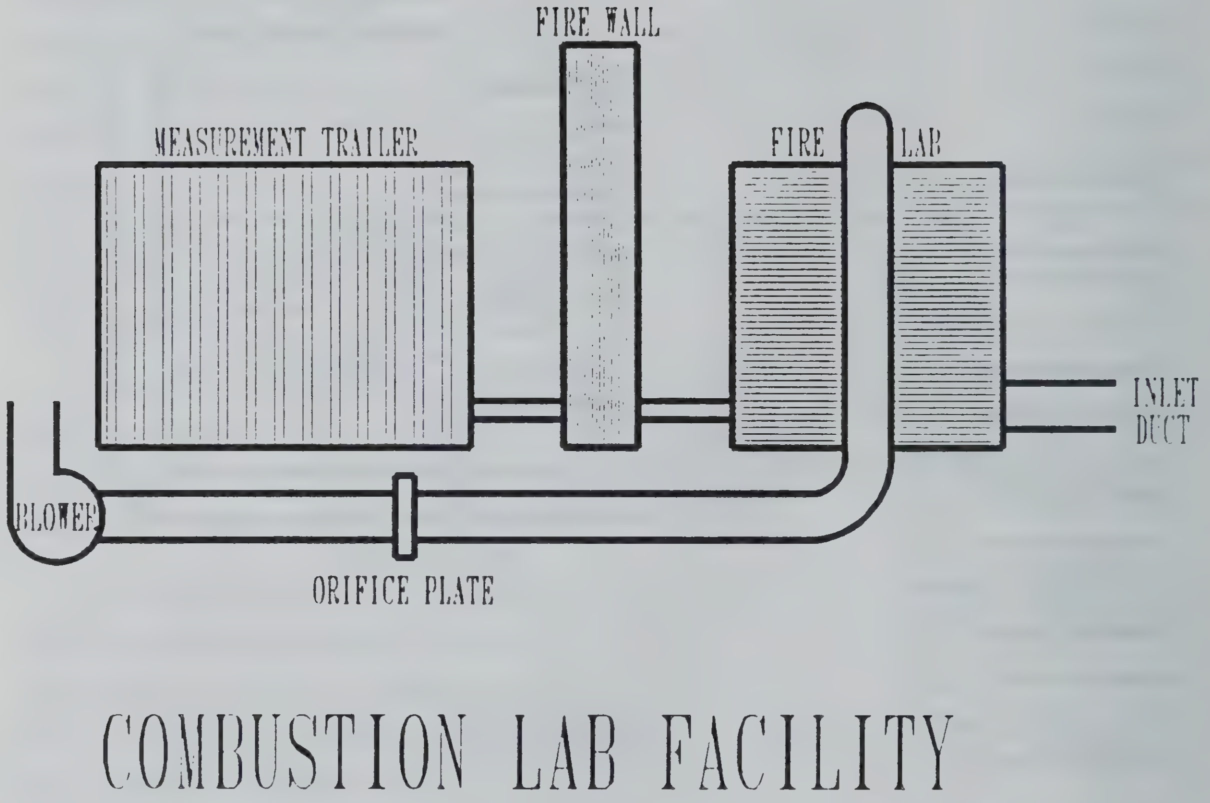


Figure 3. Combustion lab facility.

building equipped with a steel overhead door and a blowout roof. The test building is separated from the measurement trailer by a steel reinforced concrete wall. As shown in the schematic, renovation of the building has included the installation of an exhaust system. This exhaust system includes a 1.52m by 1.52m exhaust hood and the orifice meter for exhaust flow measurements.

Fabrication of the test compartment (Figure 1) was also completed in the first year. The compartment consists of an angle-iron frame with insulating ceramic board on the inside. The bottom 0.4 meters of the compartment serves as the air inlet plenum and will house a sensor for measurement of fuel weight-loss rate. The overall height of the compartment is 1.5 meters and it contains an opening which can be as large as 0.5 meters on a side. The test compartment is placed in the test building under the hood during testing. Fresh air for the compartment is drawn into the base of the compartment through a 30.5 inch inlet duct open to the outside.

Compartment Testing

After construction of the scale compartment was completed, several test burns were performed using hexane pool fires. These tests were made to determine if the compartment will function with one directional, unforced flow. These tests proved successful. A two-layer environment was achieved in the compartment using a 40 cm by 40 cm opening with an 20 cm soffit height. The fuel for the fires was supplied by a 2.5 cm deep by 22 cm in diameter pan of hexane. Total burn times were five to seven minutes. After an initial period of one to two minutes, the layer level was below the bottom of the compartment opening and flow (as indicated by smoke) was only out of the window opening. Under these conditions, there was no sustained flame out the widow; however, on one occasion a transient flame out the widow was observed just prior to fuel burn-out.

Several additional test burns were done in the compartment to test some of the monitoring instrumentation. Inlet flow velocity, CO and $CO_2$ concentrations in the layer, and the compartment temperature were measured simultaneously. These tests were conducted using a 20 cm high by 40 cm wide vent opening with a soffit height of 20 cm. A 10 cm x 20 cm hexane pool fire was used for these tests. As with the previous tests, a two layer environment was established inside the compartment with the bottom of the upper layer below the bottom of the vent opening. The air flow velocity through the 30 cm diameter inlet duct was measured at 1.2 m/s and was observed not to very by more than 5% over the steady-state portion of the tests. The steady-state CO and $CO_2$ concentrations in the layer were 500 ppm and 11.8% respectively and the peak temperature was approximately 400 C.

These results demonstrated the suitability of the compartment design for obtaining a two-layer room fire environment with no inflow in the widow. These results also demonstrated the viability of supplying air from underneath the compartment in a way that allows for measurement of compartment air inflow. The ability to carefully measure air inflow is critical to the experiments. These tests constituted a major milestone in demonstrating the suitability of the experimental design and constituted completion of the first year's objectives of the research program.

### Summary of First Year Accomplishments

First year work focused on design and development of the test compartment and the test facility. Construction of the compartment and renovation of the test facility were completed. Installation and calibration of the initial instrumentation was completed along with a gas sampling system. Several test burns performed in the compartment using hexane pool fires proved the suitability of the compartment design. The goals of the first year of the program were exceeded because some instrumentation not expected until the second year was available in the first year. As a result, the sampling system was developed ahead of schedule. This allowed detailed measurements of CO and $CO_2$ to be made earlier in the second year than originally anticipated.

In addition, a successful experimental investigation of window breakage under compartment fire conditions was completed. The study confirmed theoretical predictions by several investigators that windows break under fire conditions due to thermal stress caused by the temperature difference between the heated, exposed center of the glass and the cold, insulated edges. Windows were observed to fail catastrophically at an average temperature difference of 90C in good agreement with theoretical predictions of 60C-80C.

## SECOND YEAR ACCOMPLISHMENTS

### Additions and Modifications

Several additions and modifications were made to the experimental setup during the second year. A Siemens paramagnetic oxygen analyzer was installed on the inline measuring system. An aspirated thermocouple tree replaced the original unshielded tree of 8 thermocouples placed in the front right corner of the compartment. The aspirated tree is oriented such that the beads are facing the back wall and are 10 cm away from the side wall to avoid wall jets and boundary layer effects. A new data acquisition system and computer were added with capability to record 8 instruments and 16 thermocouples. Previously, temperature measurements were restricted to stripchart recorders. With the thermocouple capability temperature profiles in the compartment are now obtainable.

Several modifications were made to the experimental setup during the third quarter. The air flow probe was removed from the system and recalibrated upon discovering a manufacturing error. The floor of the fire compartment was covered with fire insulation board to reduce heating of the floor and plenum. The 30 second lag time in measuring the compartment sample was reduced to 10 seconds by utilizing a bypass flow.

Fluctuations in the inlet air velocity probe measurements were investigated using an FFT analysis. The velocity profile with respect to time fluctuates during some fires, particularly for fires which stay overventilated. The fluctuations are believed to be caused by the periodic air entrainment of the fire. The results of the FFT analysis are inconclusive in characterizing any dominant frequencies for either over- or underventilated fires. However, the current data acquisition system samples at 0.5 Hz which is too slow to detect plume fluctuations which are expected to be 2 to 15 Hz.

Both the CO and $CO_2$ Beckman NDIR analyzers required service for poor performance. Both are new instruments that have only been in service for about a year. Both analyzers have had their chopper motors replaced and the $CO_2$ analyzer is currently having the power supply and microprocessor board replaced. The analyzers are expected to be returned from the manufacturer in mid-September.

Total hydrocarbon measurements will be made with the addition of an FID analyzer. The major components of this were obtained during the fourth quarter and it is expected that the analyzer will be built during the first quarter of the third year. In addition, the components for a soot measurement device have been obtained and this capability will also be added to the experimental setup during the next quarter.

## HEXANE POOL FIRES

### Results

During the second year, a series of hexane pool fires were burned with four exhaust vent openings (62.5, 125, 190 and 250 $in^2$. [0.0403, 0.0806, 0.123 and 0.161 $m^2$]) and three pan sizes (32, 64, 96 $in^2$ [0.0206, 0.0413 and 0.0619 $m^2$]). All pans are 2 in (5.08 cm) deep. The goal of this work was to obtain the first complete set of data for CO yield as a function of equivalence ratio in the compartment. Hexane was chosen as a simple first fuel which had been studied previously by Beyler in a hood environment [1,2].

The various combinations of pool size and vent size yielded steady-state overall plume equivalence ratios from 0.3 to 3. All fires produced a two layer system with a uniform upper layer which has been verified with temperature and species concentration measurements. As a result of the uniform upper layer, sampling was not dependant on probe location. Thus, sampling was performed with an uncooled stainless steel probe centered in the exhaust vent 12 cm into the compartment.

Results from two typical fires are shown in Figures 4 and 5. Figure 4 is a typical overventilated fire. The equivalence ratio remained below 1.0 throughout the entire experiment. The fire was ignited at time zero. The $CO_2$ concentration rises quickly in the first 60 seconds and then increases more slowly for the next 5 minutes. As expected under such conditions, the generation rate of CO was quite small leading to CO concentrations of less than 0.05 percent throughout the entire experiment. As the compartment approaches the underventilated condition (equivalence ratio of one) the $CO_2$ concentration increases sharply and the $O_2$ concentration decreases sharply but only to 9 percent, whereas $O_2$ concentrations are less than 0.5 percent for underventilated fires. The large increase in the equivalence ratio near the end of the fire is due to a rapid increase in the fuel volatilization rate just prior to burnout. This is a commonly observed behavior for pool fires in metal pans. At steady-state, the fire obtained an equivalence ratio of 0.65 and a fuel volatilization rate of 1.8 g/s for approximately one minute during this test.

Figure 5 shows the results from a typical underventilated fire. In this test, there is also an initial rapid rise observed in $CO_2$ at the start of the test. However, the rise in $CO_2$ with time is greater than in the test shown in Figure 4 due to the higher compartment temperatures, resulting from the higher equivalence ratio early in the test. At approximately 115 seconds the compartment fire transitions from an over- to underventilated condition. During this transition the fire changes from a localized fire to one with flames emerging from the opening. This behavior is typical of under-ventilated compartment fires and is consistent with the interpretations of flashover as a thermal instability. It should be noted that this "flashover" phenomenon as shown by the rapid increase in the $CO/CO_2$ concentrations was accompanied by a dramatic increase in the volume of smoke emerging from the vent and then by sustained external burning. External burning is burning of upper-layer combustion products that are ignited outside of the compartment by the entrainment of ambient air. Sustained external burning occurs at an equivalence ratio of one or higher. Prior to an equivalence ratio of one, external burning occurs as a flash phenomenon. In contrast to these results Beyler did not observe external burning until an equivalence ratio of 1.8. Very little smoke and no external burning were observed during the overventilated fire of Figure 4.

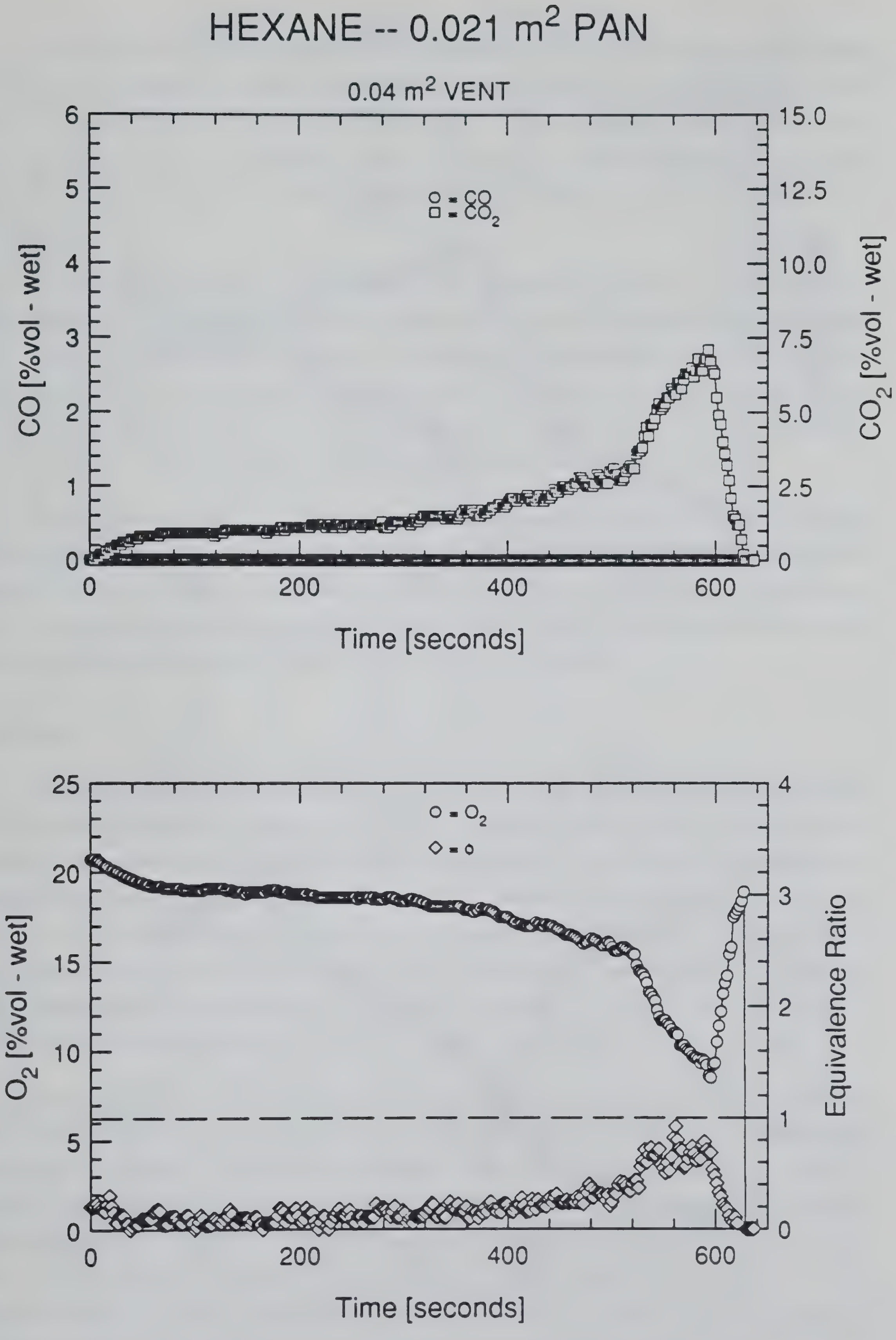


Figure 4. Typical Overventilated Hexane Fire

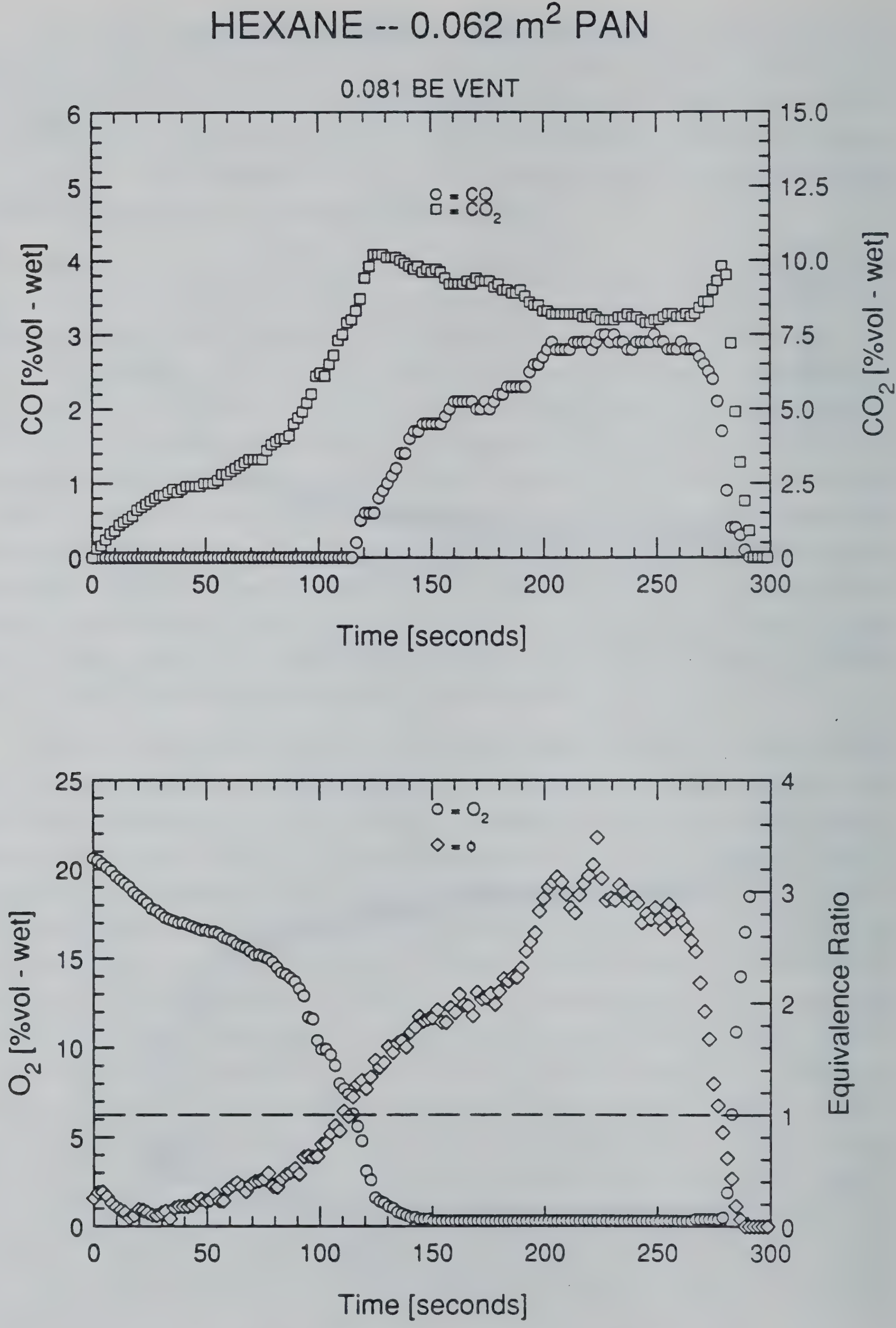


Figure 5. Typical Underventilated Hexane Fire

Prior to the transition to underventilated conditions CO concentrations are less than 0.05% as in the fires that remain overventilated. As the Equivalence ratio increases beyond 1.0, the CO concentration begins to increase rapidly, reaching lethal levels of 3% in this case. The $O_2$ concentration decreases sharply at the onset of transition and levels out below 0.5%. This fire obtained a steady-state average equivalence ratio of 3.1 and a fuel volatilization rate of 15 g/s.

The $O_2$ concentration for the hexane tests decreased to below 1 percent for the underventilated fires and reached steady state values below 0.05 percent for several tests. These small $O_2$ concentrations are lower than expected based on Beyler's results. Beyler observed minimum $O_2$ concentrations of 3 percent for equivalence ratios from 0.3 to 1.6. The difference is assumed to be due to the unrestricted amount of air available to Beyler's hood setup. In the closed compartment the oxygen is consumed more completely.

The $CO_2$ concentration reaches a maximum when the fire reaches an equivalence ratio slightly larger than one. As the equivalence ratio increases the CO concentration rises and the $CO_2$ concentration decreases to a steady-state value. The $CO_2$ concentrations are lower than expected due to an unsystematic drift in the analyzer. The analyzer was returned to the manufacturer for repair during the end of the fourth quarter.

## Discussion

A carbon balance analysis was performed to verify that all carbon introduced into the system was accounted for properly. All carbon originates from the fuel. The fraction of unburned hydrocarbons produced for equivalence ratios greater than one is a function of equivalence ratio according to the expression $1 - 1/\Phi$. This expression was verified by Beyler in his experiments by measurement of unburned hydrocarbons. The fraction of carbon not accounted for by the CO and $CO_2$ concentrations was calculated and compared to the fraction of carbon expected as unburned hydrocarbons. As can be seen in Table I, the carbon balance obtained based on the above assumption is good.

The experimental steady-state concentrations of CO and $CO_2$ differ significantly from equilibrium thermodynamic concentrations. STANJAN, a thermodynamic equilibrium program, was used to calculate CO and $CO_2$ concentrations for fire temperatures ranging from the upper layer temperature to the adiabatic flame temperature. Thermodynamics consistently overpredicts the CO concentration by as much as 5 to 10 times the experimental results for equivalence ratios greater than one. The $CO_2$ concentrations are underpredicted by as much as one half of the experimental steady-state average values for fuelrich conditions. The transient dynamics of the compartment fire

Table I. Carbon Balance

| Carbon Error | 1-1/Phi |
|---|---|
| 0.33 | 0.21 |
| 0.42 | 0.22 |
| 0.34 | 0.28 |
| 0.32 | 0.34 |
| 0.35 | 0.35 |
| 0.43 | 0.44 |
| 0.48 | 0.48 |
| 0.56 | 0.57 |
| 0.6 | 0.63 |
| 0.62 | 0.64 |
| 0.64 | 0.65 |
| 0.67 | 0.67 |

obviously prevent thermodynamic equilibrium from occurring. The residence time is approximately 30 seconds which is too short to allow approach to equilibrium at the observed upper layer temperatures.

A study was undertaken to develop a relationship between the experimental and theoretical CO concentrations. Figure 6 shows experimental and thermodynamic equilibrium CO concentrations verses equivalence ratio for a range of temperatures. Several notable observations can be made. By applying a gain of 7 to 7.5 to the experimental data, fairly close agreement can be made between thermodynamic and experimental CO concentrations. For equivalence ratios less than 1.5 agreement is better for temperatures below 2000 K. For equivalence ratios greater than 1.5 agreement is better for temperatures above 2000 K for which the equilibrium concentrations converge to within 1.5 percent. The maximum deviation of the experimental data to the thermodynamic equilibrium concentrations is within 18 percent for equivalence ratios greater than 1.8. As will be discussed next, an equivalence ratio of 1.8 denotes the point at which CO yield reaches a constant value.

The hexane experiments show a distinct correlation between the species yield and the overall equivalence ratio. Yield is the grams of species produced per gram of fuel burned. The overall equivalence ratio is the ratio of fuel volatilization rate to air entrainment rate normalized by the stoichiometric fuel-to-air ratio. The $O_2$ yield is the grams of oxygen consumed per gram of fuel burned. The steady-state average yield is plotted versus the steady-state average equivalence ratio for all fires in Figures 7 and 8.

Figure 7 shows two plots: CO yield with respect to equivalence ratio and $CO_2$ yield with respect to equivalence ratio. As can be seen, the correlations are similar to the correlations obtained from Beyler's hood experiments. Beyler's hood experiments differed in several ways from actual compartment fires. The setup had a forced exhaust system and an infinite supply of air which was neither vitiated nor heated by vent flow mixing. Beyler was also able to sustain a steady-state environment. The current experiments involve only buoyancy driven flows and a limited supply of air to the fire. The air which is entrained into the compartment lower layer is convectively heated by the hot compartment surfaces prior to fire plume entrainment. Currently no measurements have been made of the oxygen concentration in the lower layer to determine the extent to which it is vitiated. The hexane fires are primarily transient experiments with short steady-state periods. During the steady-state periods of the fires, large ceiling and wall jets are present for high equivalence ratio fires. Beyler's hood experiments did not include these dynamic flame structures which enhance mixing of the layer. Despite the differences in experiments the yield-equivalence ratio correlations agree fairly well.

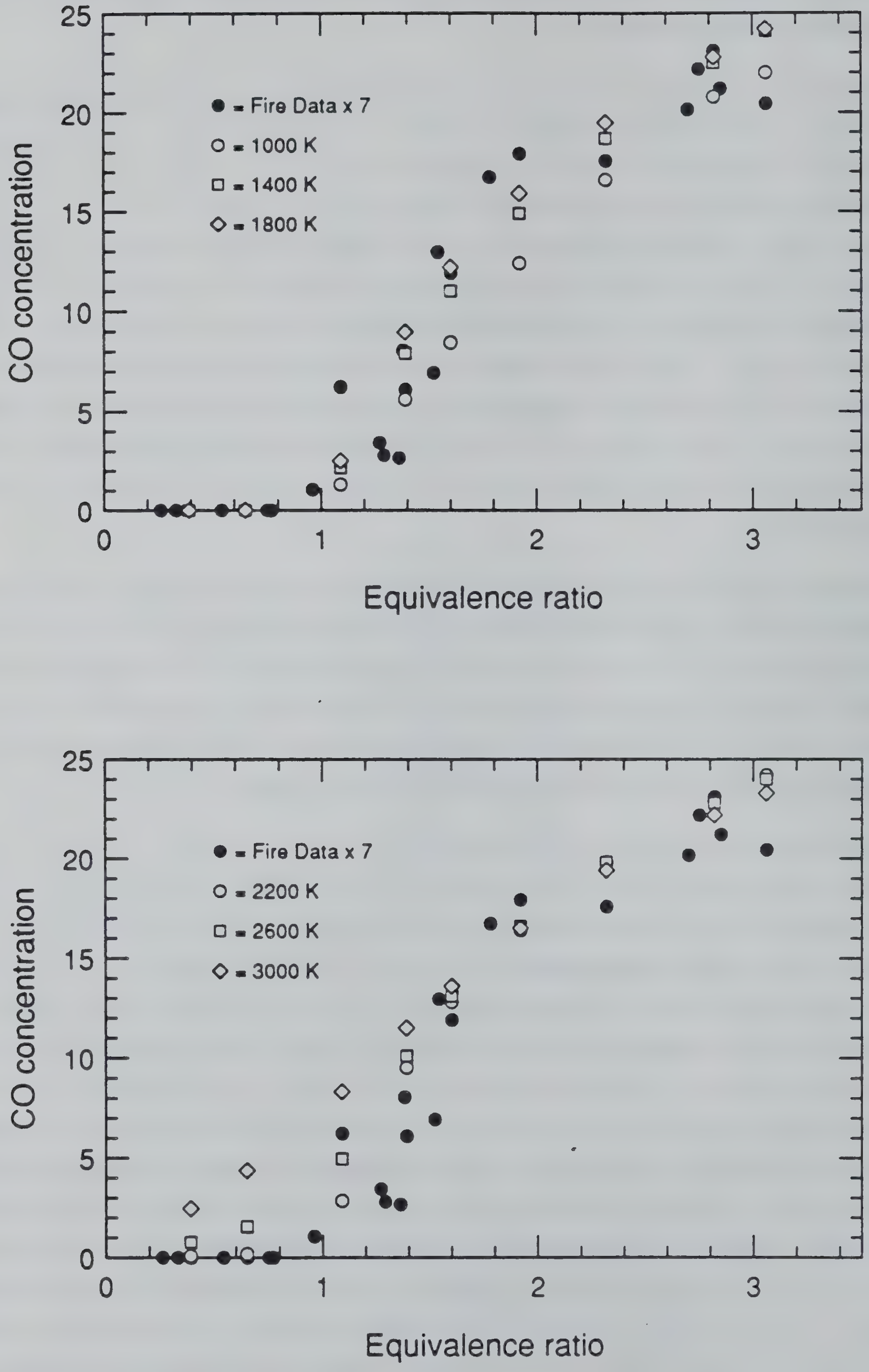
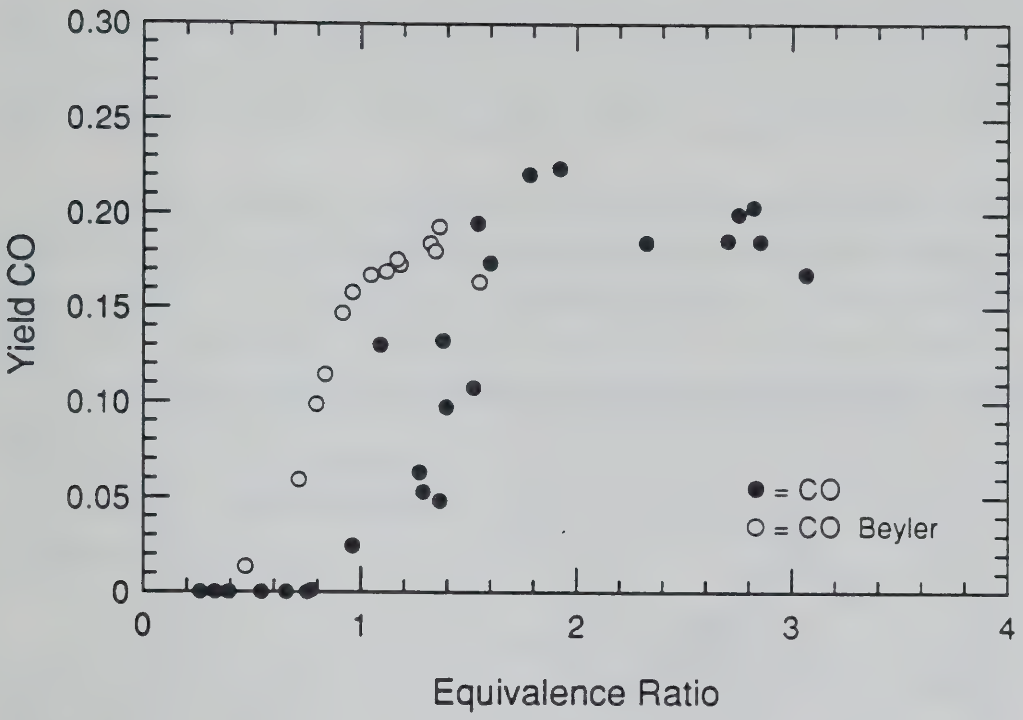


Figure 6. Thermodynamic Equilibrium [CO]



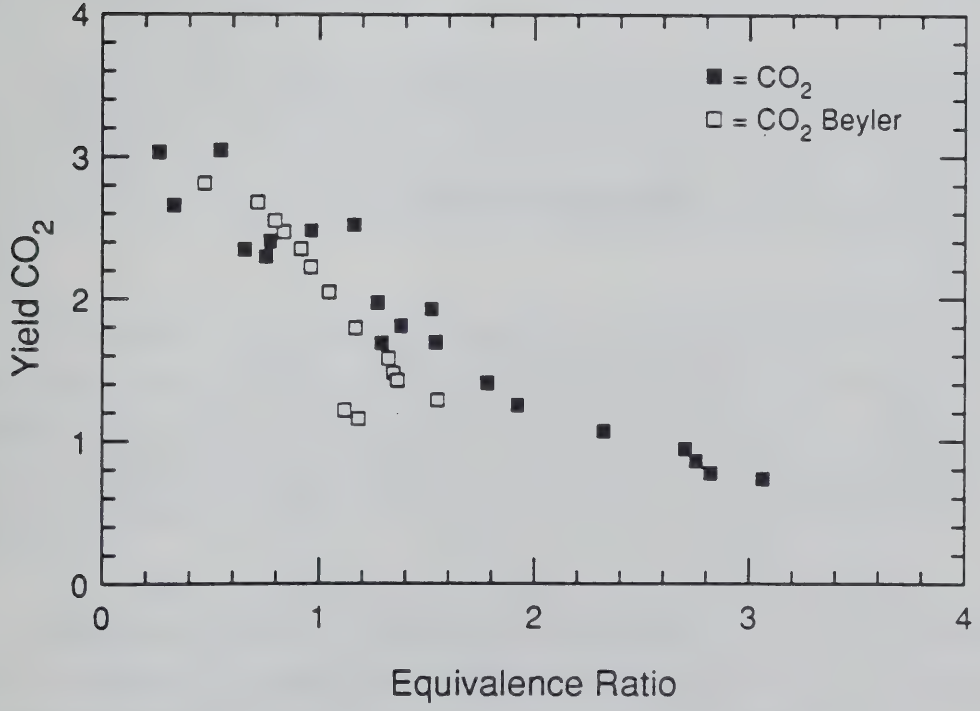


Figure 7. Steady-state Yield - Equivalence Ratio

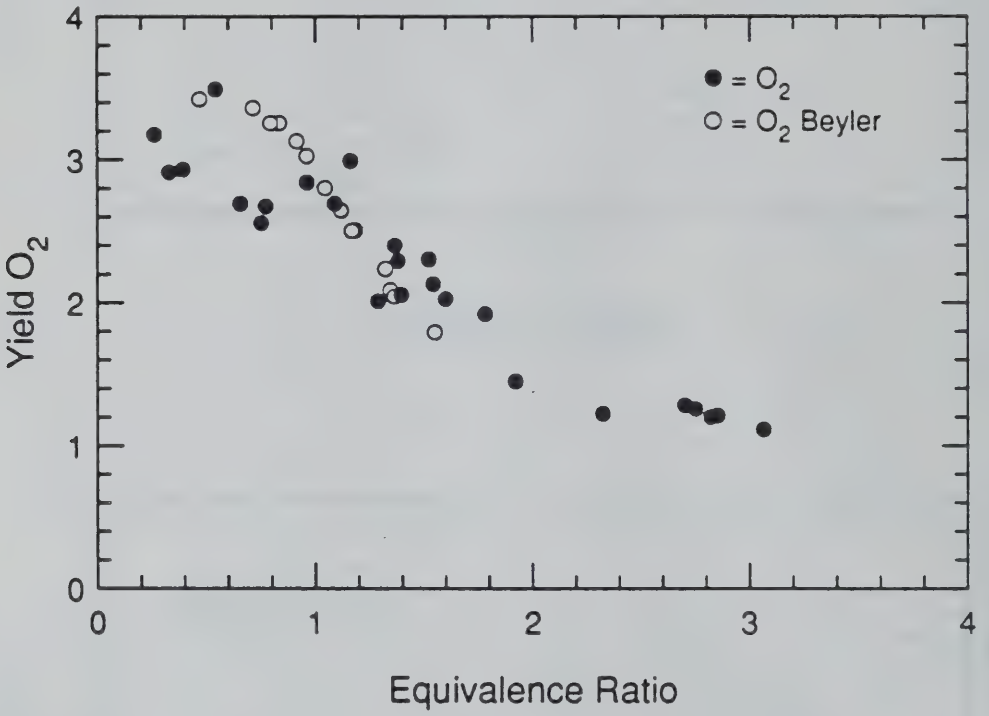


Figure 8. Steady-State Yield - Equivalence Ratio

The top plot of Figure 7 shows an offset between Beyler's rise in CO yield and the results of these tests. Beyler's experiments show the CO yield rising before an equivalence ratio of one where as the current results do not show the CO yield rising until an equivalence ratio of one. The cause of this offset is not known, but may be attributed to the more realistic conditions in these compartment fires compared to Beyler's hood setup.

As seen in Figure 7 the CO yield correlated with the equivalence ratio exhibits a primarily two-value function with a transition region between equivalence ratios of 1 and approximately 1.8. At equivalence ratios greater than 1.8 a leveling off of CO yield is observed at approximately 0.20. The $CO_2$ yield-equivalence ratio shows a two-value function similar to that observed for CO; however, the $CO_2$ yields are high at low equivalence ratios and low at high equivalence ratios. Similar to the CO correlation, the $CO_2$ correlation seems to be somewhat offset from Beyler's result. Figure 8 shows the $O_2$ yield-equivalence ratio correlation. Similar to the CO yield, the $O_2$ yield levels out at equivalence ratios greater than 2 to a value of 1.2.

Hexane fires with steady-state equivalence ratios of 2 or greater exhibit transient yield to equivalence ratio correlations similar to the steady-state correlations. A transient correlation is obtained from the transient data of one fire where as the steady-state correlation is obtained by using the steady-state value from each fire. Figure 9 and 10 show the transient correlations for the underventilated fire shown in Figure 5. The fire had a steady-state equivalence ratio of 3.1.

The top plot of Figure 9 shows the same correlation between CO yield and equivalence ratio as seen in the steady-state correlation in Figure 7. The CO yield is essentially zero until an equivalence ratio of one is reached. The CO yield increases during the transition region, equivalence ratio of 1 to 2, and then levels out to a relatively constant value.

The multiple $CO_2$ and $O_2$ yield points at an equivalence ratio of 0.2 are actually increasing in time as the fire is started and burns for the first 60 seconds. The initial low values in $CO_2$ and $O_2$ yield are due to the initial volume of air in the compartment which is not accounted for in these yield values. As expected the $O_2$ yield (consumption) is larger in the over-ventilated condition and decreases with the transition to the under-ventilated condition.

Temperature profiles at three different times in an over- and underventilated fire are shown in Figure 11. Temperature measurements are made with a tree of eight aspirated thermocouples located in the front right corner of the compartment. For the purpose of

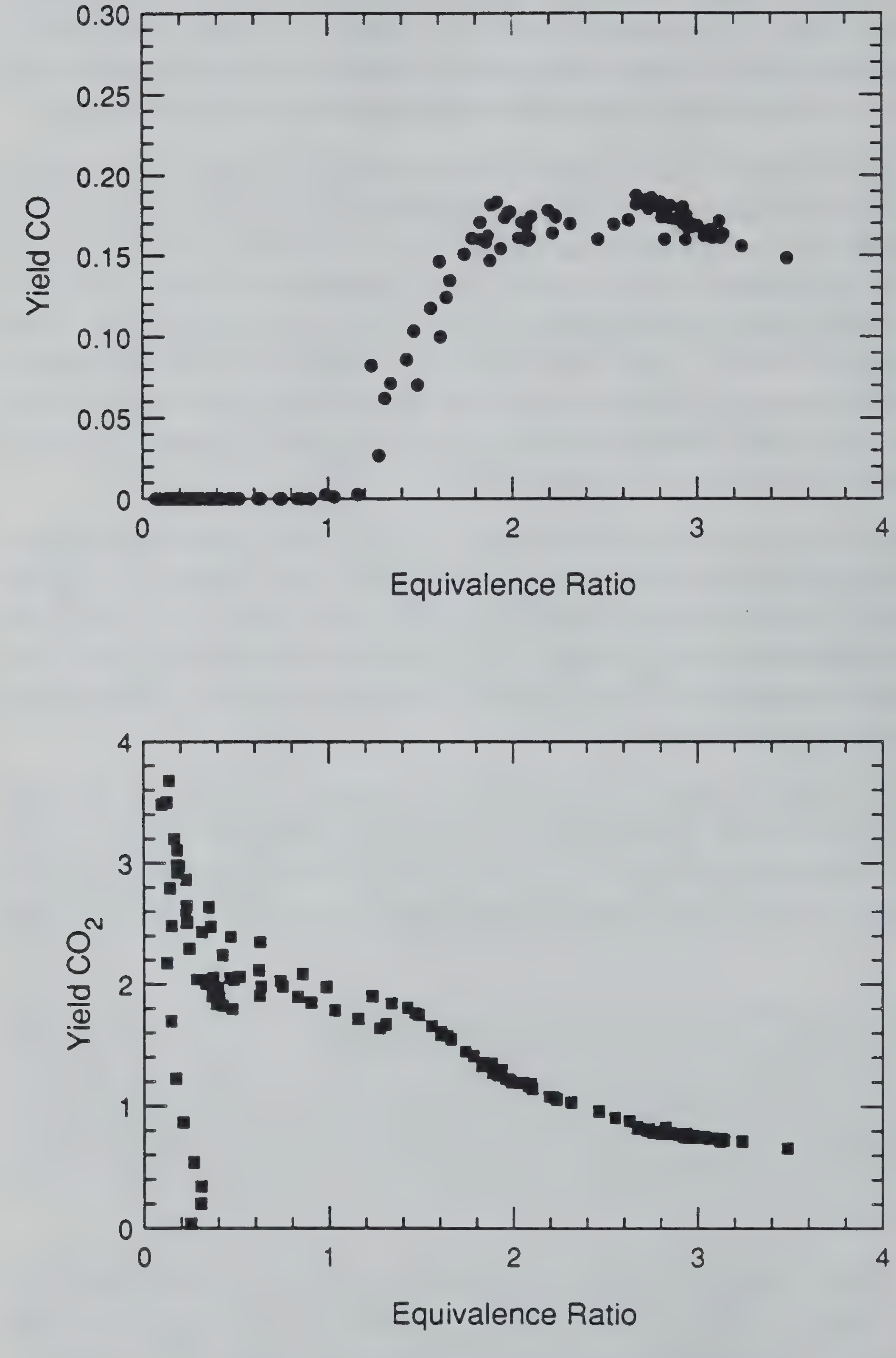


Figure 9. Transient Yield - Equivalence Ratio

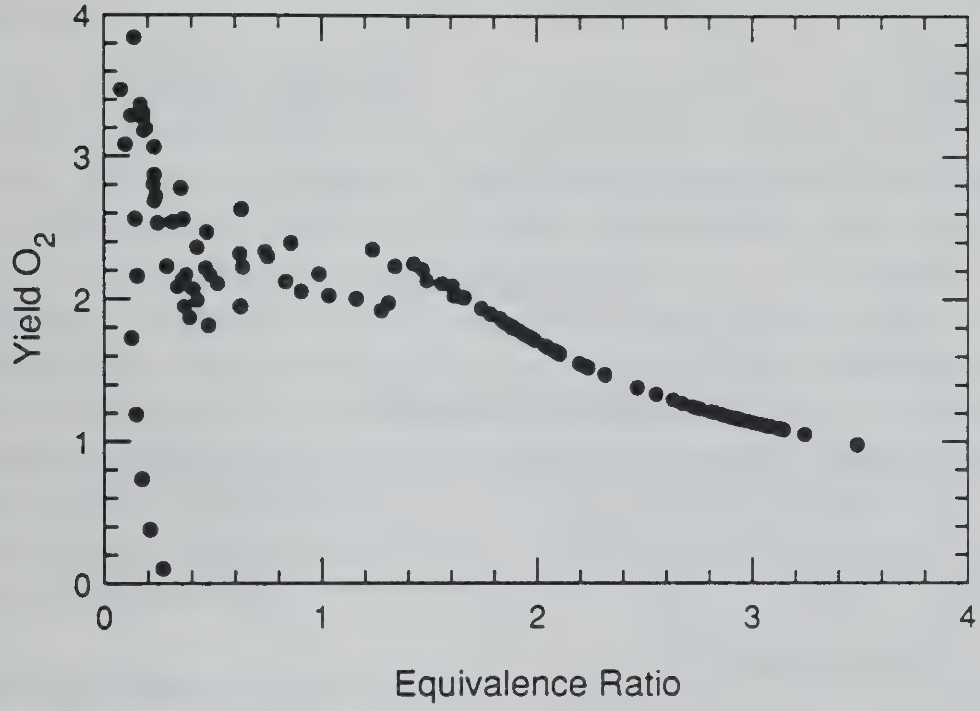
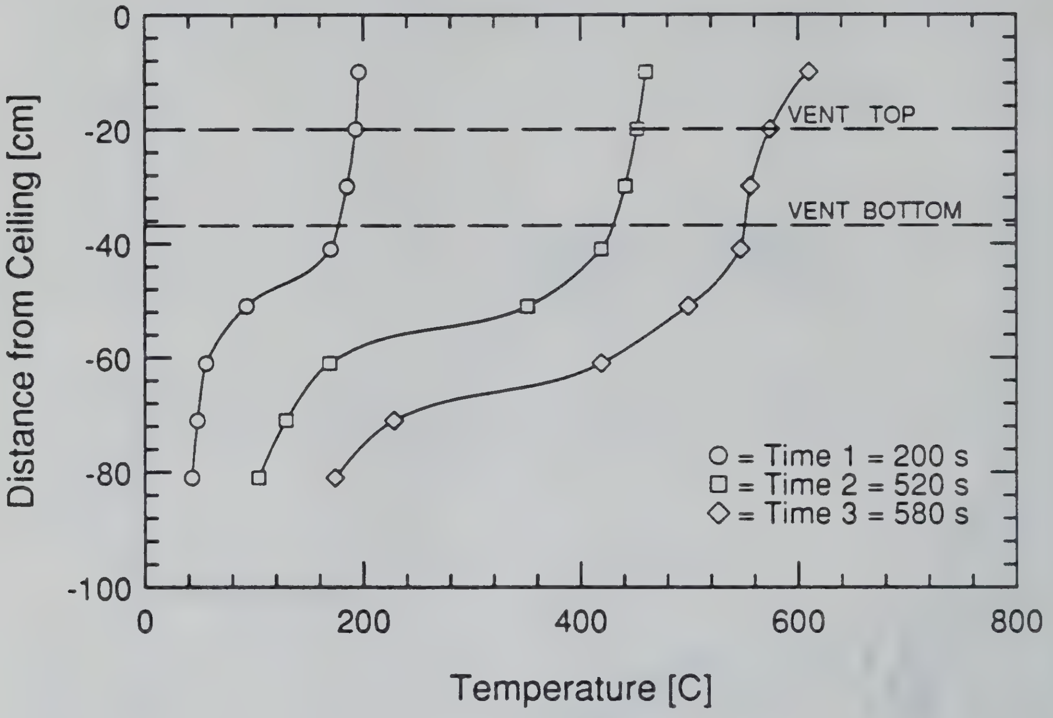


Figure 10. Transient Yield - Equivalence Ratio

Overventilated Fire



Underventilated Fire

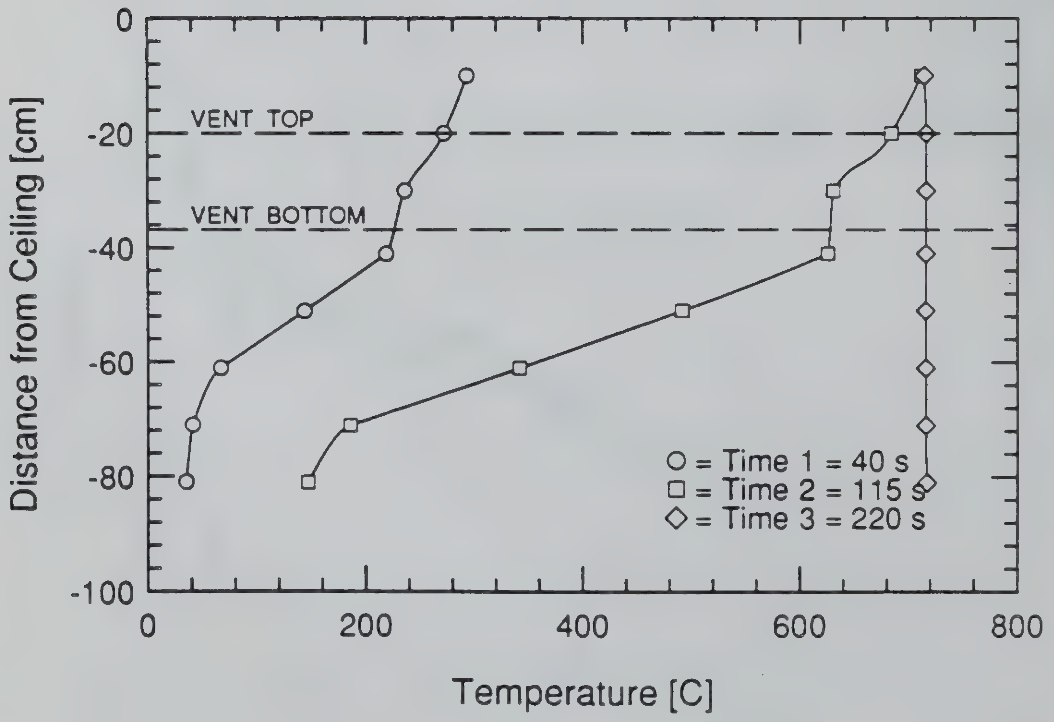


Figure 11. Temperature Profiles for Hexane Fires

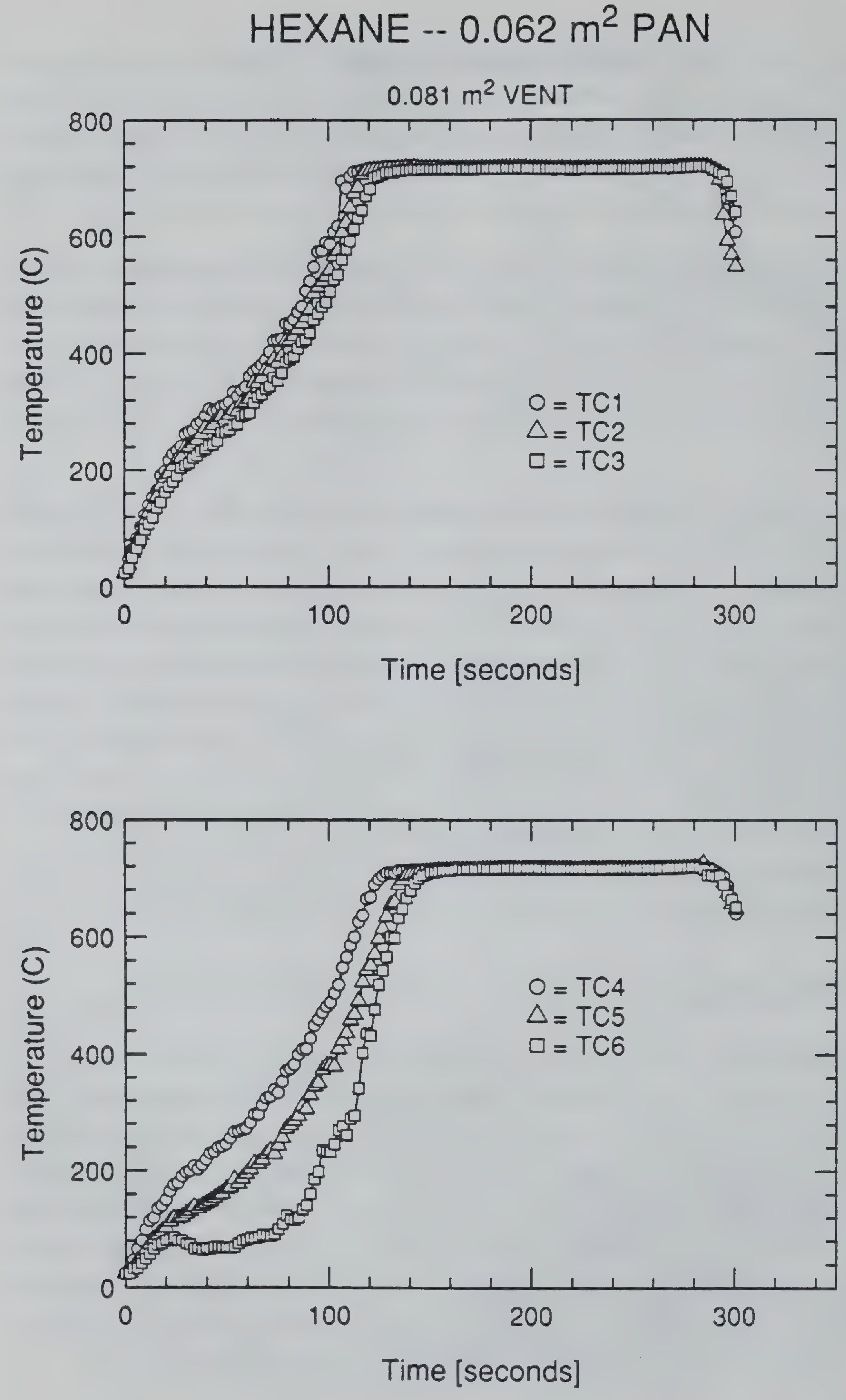
comparison the same over- and underventilated fires shown in Figure 4 and 5 are used in Figure 11. As can be seen a distinct thermal layer develops in both the over- and underventilated fires and quickly reaches a depth that is below the vent opening. However, the upper layer develops faster in the underventilated fire and reaches a depth greater than 81 cm.

The layer interface is assumed to be midway between the thermocouple positions showing the sharp drop in temperature from the relatively uniform upper layer to the cooler lower layer of air. Approximately a 100 C temperature difference exists between the upper layer of hot gases and the lower layer for the underventilated fire. The steady-state period of the underventilated fire is marked by the uniform temperature profile of 720 C in the upper layer.

Figure 12 shows transient temperature profiles of the underventilated fire shown in Figure 11. Note that the thermocouples are numbered from 1 at the top to 8 at the bottom of the tree. The transient temperature plots of the thermocouples bordering the large temperature gradient (TC4 and TC5) show little fluctuation in temperature and, therefore, suggests that any mixing of the upper and lower layers occurs in an interface less than the thermocouple spacing of 10 cm. Based on this observation, the layer interface is assumed to be relatively stable with little mixing. A narrow window will be installed down the side of the compartment in order to make visual observations of the layer during future experiments. Thermocouples 1 to 3 show a layer that is relatively uniform throughout the fire. The transition from an over- to underventilated condition occurred at 115 seconds (see Figure 5) which corresponds to the time at which the upper layer reaches the maximum steady-state value of 720 C.

## Summary of Hexane Fires

The hexane-fueled fires produce a two-layer system with a uniform upper layer which has been verified with temperature and species concentration measurements. The layer interface thickness appears to be less than 10 cm. The transition from an overventilated (equivalence ratio below one) to an underventilated fire condition is marked by several characteristics: 1) a sharp rise in CO and $CO_2$ concentrations in the upper layer, 2) a sharp decrease in $O_2$ concentration in the upper layer and 3) sustained external burning. Sustained external burning begins at an equivalence ratio of one. Prior to an equivalence ratio of one, external burning occurs as a flash phenomenon. In contrast to these results Beyler did not observe external burning until an equivalence ratio of 1.8.



HEXANE -- 0.062 $m^2$ PAN

0.081 $m^2$ VENT

Figure 12. Transient Temperature Profiles

The hexane experiments show a distinct correlation between the species yield and the overall equivalence ratio. The CO yield correlated with the equivalence ratio exhibits a primarily two-value function with a transition region between equivalence ratios of 1 and approximately 1.8. At equivalence ratios greater than 1.8 a leveling off of CO yield is observed at approximately 0.20. Hexane fires with steady-state equivalence ratios of 2 or greater exhibit transient yield to equivalence ratio correlations similar to the steady-state correlations.

Thermodynamics cannot predict CO and $CO_2$ concentrations observed in the hexane-fueled compartment fires. However, by applying a gain of 7 to 7.5 to the experimental data fairly close agreement can be made between thermodynamic equilibrium and experimental CO concentrations. For equivalence ratios less than 1.5 agreement is better for equilibrium temperatures below 2000 K. For equivalence ratios greater than 1.5 agreement is better for temperatures above 2000 K. The maximum deviation of the experimental data to the thermodynamic equilibrium concentrations is within 18 percent for equivalence ratios greater than 1.8.

### PMMA

Initial tests of cast PMMA slabs were performed during the fourth quarter. PMMA samples burned consisted of 0.95 cm (3/8 inch) and 1.9 cm (3/4 inch) thick 20x20 cm (8x8 inch), 30x30 cm (12x12 inch) and 38x38 cm squares. Two vent sizes were used, 0.0403 $m^2$ (62.5 $in^2$) and 0.0806 $m^2$ (125 $in^2$), in the tests performed. The PMMA sheets were ignited by igniting hexane-soaked PMMA shavings that were evenly piled on top of the sheet approximately half an inch high. The chips were soaked in hexane to assure a rapid uniform ignition over the whole surface of the PMMA sheet and, thus, decreasing the time to steady-state burning.

The initial tests repeat several of the conclusions observed from the hexane tests: temperature profiles show the establishment of a two layer system and overventilated fires show no CO and no external burning. Oxygen concentrations of 9 to 17 percent have been observed for the tests performed.

Figure 13 shows CO, $CO_2$ and $O_2$ concentrations for a typical overventilated PMMA fire that reached a steady-state equivalence ratio of 0.5. This fire condition was obtained using a 1.9 cm thick 38x38 cm sheet of PMMA with a 0.0806 $m^2$ vent. Similar to the hexane results the $O_2$ concentration is quite high for the overventilated fire and the CO concentration is below 0.05 percent. As this fire approached the transition to an underventilated condition the $O_2$ concentration sharply decreased while the $CO_2$

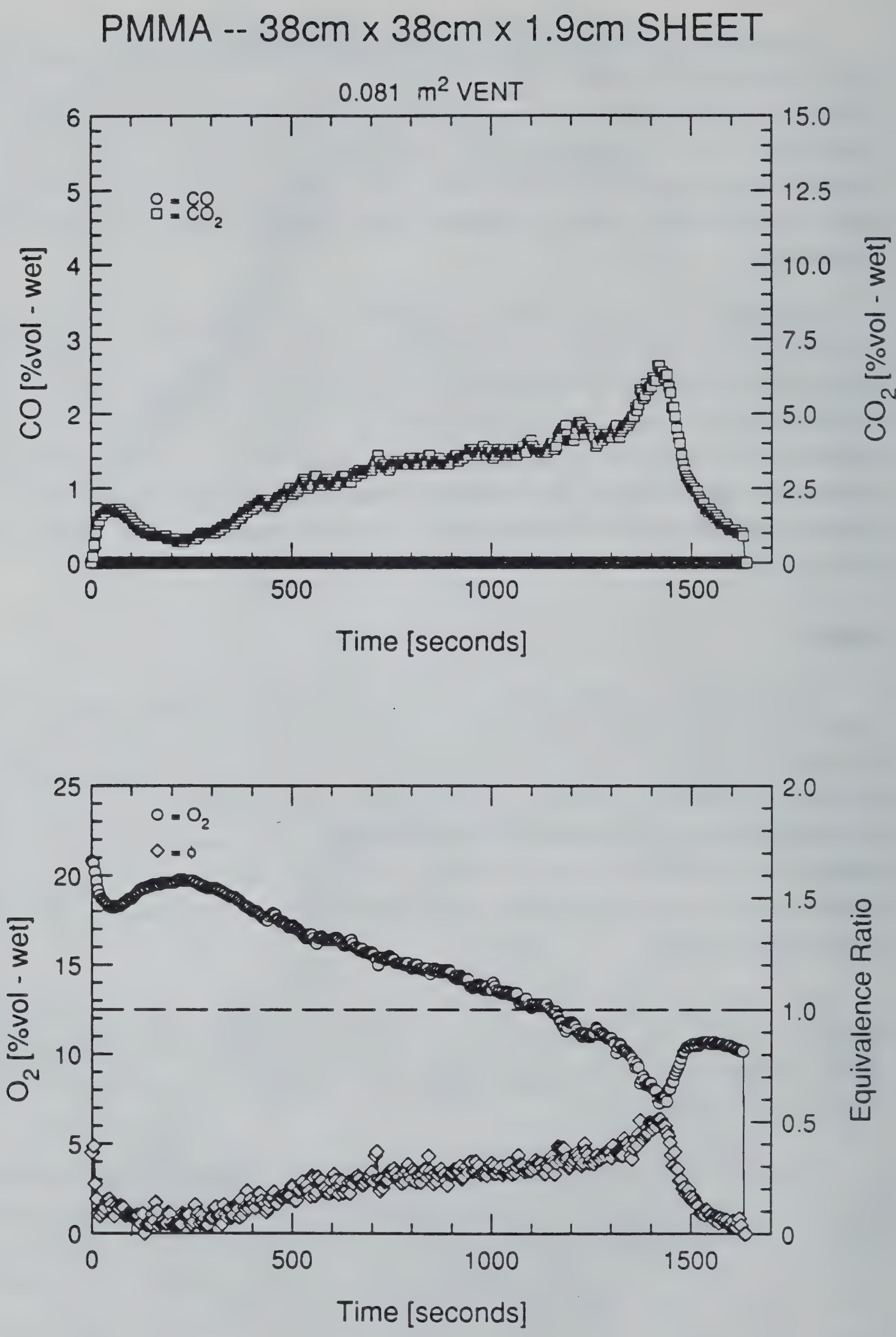


Figure 13. Typical Overventilated PMMA Fire

concentration sharply increased. As expected, these PMMA results show transition characteristics similar to those of the hexane fires.

Figure 14 shows CO, $CO_2$ and $O_2$ concentrations for a typical overventilated PMMA fire that reached a steady-state equivalence ratio of 1.6. This fire condition was obtained using a 1.9 cm thick 38x38 cm sheet of PMMA with a 0.0403 $m^2$ vent. Similar to the hexane-fueled fires the CO concentration remains below 0.05 percent and increases sharply as the fire becomes underventilated. During this transition the $O_2$ concentration decreases to near zero and the $CO_2$ concentration rises sharply to a steady-state value of 14.3 percent.

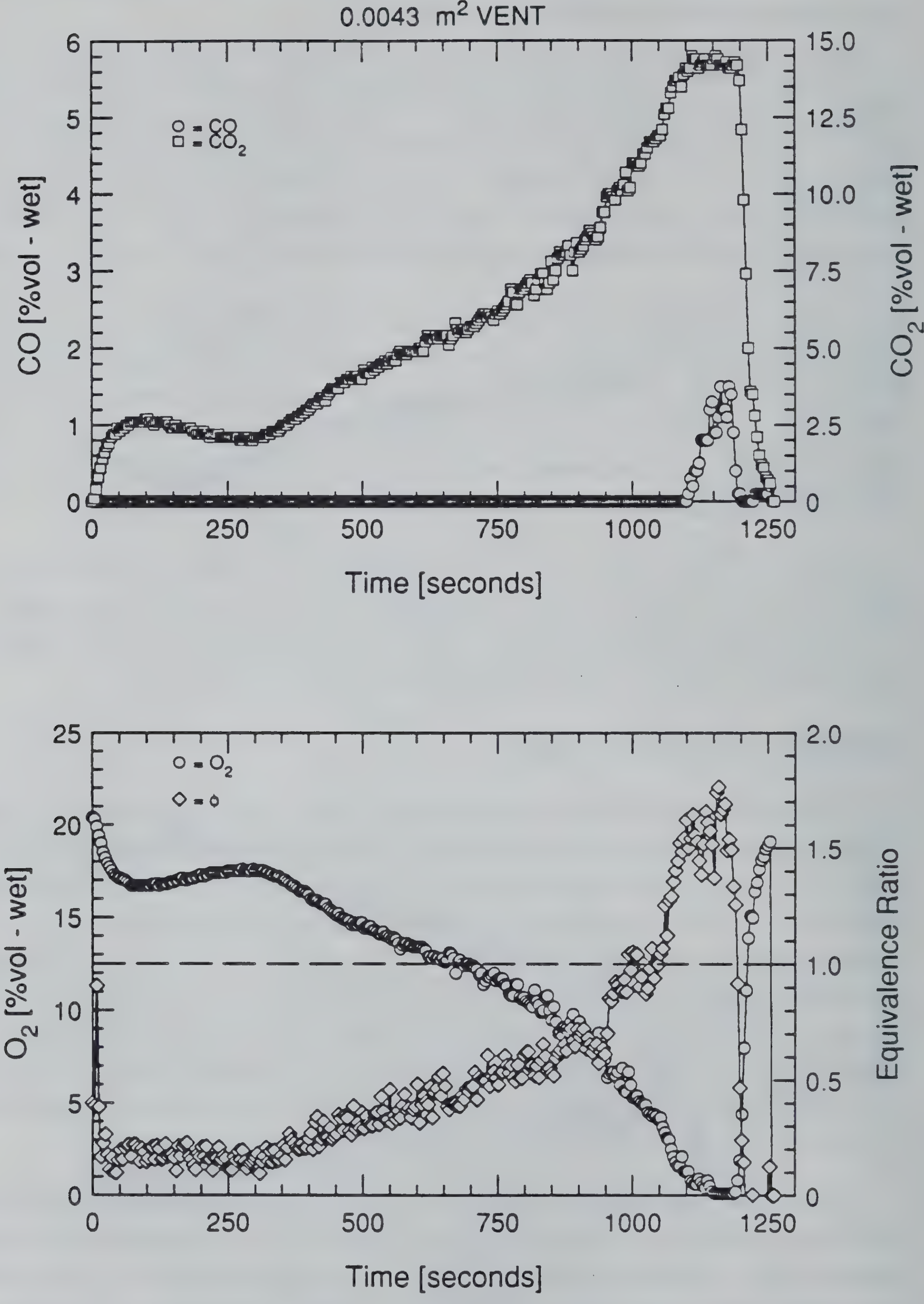
Figure 15 shows a typical temperature profile for a PMMA fire. The steady-state equivalence ratio is one for the fire shown. The temperature profile indicates the formation of a two layer system. The upper layer reaches a steady-state temperature of approximately 480 C with a layer over 80 cm deep. The PMMA fires produce more soot than the hexane fires. The slightly lower temperatures at the top of the layer is believed to be caused by a tendency for the higher thermocouples to be coated with soot later in the fire.

Further PMMA-fueled fires will be performed in order to develop yield to equivalence ratio correlations. The various species correlations are expected to agree well with the correlations obtained from the hexane-fueled fires once the yields are normalized by the maximum theoretical yield of those species for the fuel used.

## SUMMARY AND FUTURE WORK

During the second year several modifications were made to the experimental setup, an oxygen analyzer and a new data acquisition system with thermocouple capability were added, a bypass flow was created to reduce sampling time lag, additional insulation was used on the floor of the compartment to reduce heating of the floor and plenum and the air velocity probe was recalibrated. The noise in the velocity probe has been eliminated. Fluctuations in the inlet air velocity have been observed, however, an FFT analysis of the data was inconclusive in characterizing any dominant frequencies for either under- or overventilated fires. Both the CO and $CO_2$ Beckman NDIR analyzers required service for poor performance and are expected to be returned from the manufacturer in early in the first quarter of the third year.

The hexane yield-equivalence ratio correlations agree well with Beyler's results. The CO yield correlates with the equivalence ratio primarily as a two-value function with a transition region between equivalence ratios of 1 and approximately 1.8. At equivalence ratios greater than 2 a leveling off of the yields is observed. Hexane fires with steady-state



PMMA -- 38cm x 38cm x 1.9cm SHEET

0.0043 m$^2$ VENT

Figure 14. Typical Underventilated PMMA Fire

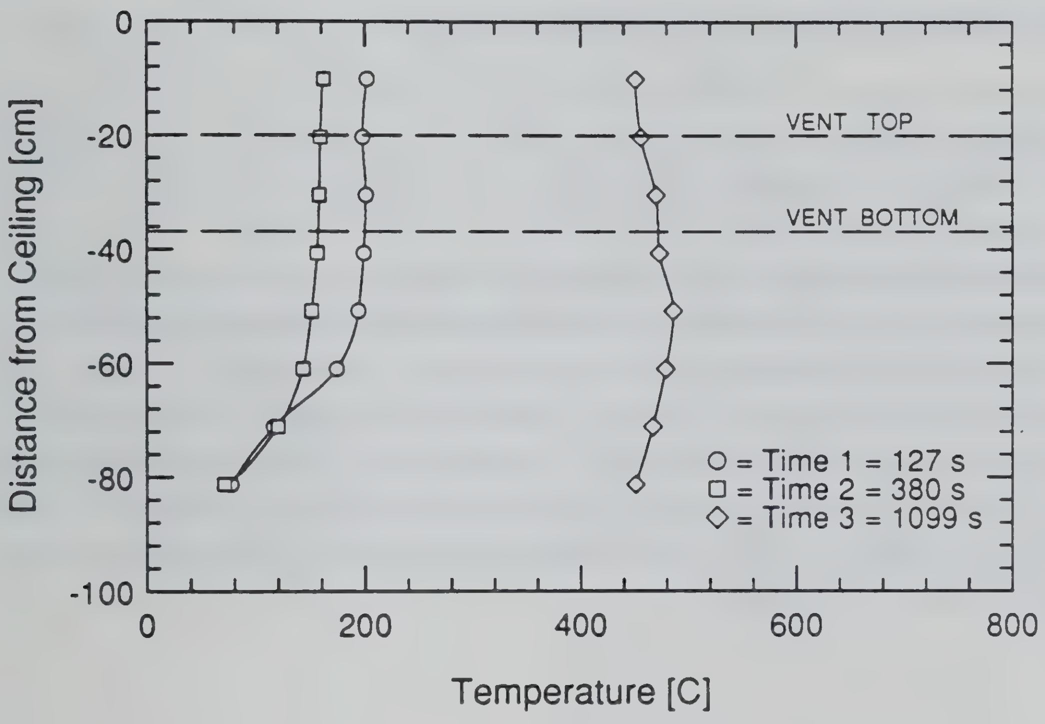


Figure 15. Temperature Profiles for a PMMA Fire

equivalence ratios of 2 or greater exhibit transient yield to equivalence ratio correlations similar to the steady-state correlations. A correlation between CO/$CO_2$ yields and equivalence ratio for transient fires provides important information for fire modeling.

The transition from over- to underventilated conditions is marked by a number of phenomena: CO yield increases sharply from zero, $CO_2$ concentrations increase dramatically, $O_2$ concentrations decrease sharply, the upper layer reaches a maximum steady-state value and sustained external burning begins. CO concentrations as high as 3.5 percent have been observed for underventilated fires. Oxygen concentrations observed for underventilated tests decrease to below 0.05 percent for several tests and below 1 percent for all equivalence ratios above 1. These concentrations are lower than the 3 percent minimum observed for Beyler's hexane hood experiments.

The third year will concentrate on completing PMMA, polyurethane and wood studies and determining the efficiency of external flames in destroying major toxic gases produced within the compartment during oxygen deficient combustion. Attempts will be made to destroy the two layer system in order to test the robustness of the yield to equivalence ratio correlation. Two configurations will be used to examine the effect of external flames on ultimate species yields. One configuration will simulate a window vent where the flame will be allowed to flow up the side of the outside wall. This is the configuration currently being used. A second configuration will use a "ceiling" outside the vent to force the flame to flow horizontally. This configuration, similar to the flame issuing into a corridor, should allow for much lower rates of entrainment of outside air. Total hydrocarbon measurements will be made upon the addition of an FID analyzer and a soot measurement device will be added.

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The interim findings of a planned three-year experimental investigation are summarized. The investigation is designed to determine the effect of realistic compartment fire flows on species production rates and their correlation with equivalence ratio and to establish major toxic gas and smoke generation rates for important fuels such as PMMA, wood and TDI-based polyurethane. The apparatus for the measurements is described and findings for a series of hexane fires over a range of equivalence ratio are described. Preliminary measurements using PMMA-fueled fires are also included.

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compartment fires; hexanes; polymethylmethacrylate; polyurethanes; smoke generation; species concentrations; toxic gases; wood

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